Magnetic tunnel junctions with impurities

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Abstract: The influence of impurities, embedded into the isolating spacer ($\mathbb{I}$) between two ferromagnetic electrodes ($\mathbb{F}$), on the I-V curve and tunnel magnetoresistance (TMR), is theoretically investigated. It is shown, that the current and TMR are strongly enhanced in the vicinity of the impurity under the condition that the energy of the electron's bound state on the impurity is close to the Fermi energy. If the position of the impurity inside the barrier is asymmetric, e.g. closer to the one of the interfaces $\mathbb{F}/\mathbb{I}$ the I-V curve exhibits quasidiode behavior.

The magnetic tunnel junction (TMJ), consisting of two metallic ferromagnetic electrodes separated by insulating barrier and exhibiting tunnel magnetoresistance (TMR) of order 50% attracts a lot of attention [1, 2, 3] especially due to their possible application in MRAM (Magnetic Random Access Memory). In the pioneer paper [4] the theory of TMR for the ideal (without defect) TMJ was developed. Later it was shown [5, 6] that in presence of different types of defects within the barrier the I-V current and TMR change dramatically. In these papers the averaged over cross section of the system current was calculated. However it is interesting to investigate the local (in vicinity of the impurity) current and TMR, especially taking into account that using the STM technique it is possible and was realized [7] to span tunnelling current over the cross section of TMJ. Recently the theory of local impurity assisted tunnelling in TMJ was developed [8]. As a model of TMJ was taken tight binding model and Kubo formalism was used for calculation of spin-dependent tunnel current. In this paper the I-V curve was not investigated in detail and besides that the dependence of spin-dependent current on the position of cross section plane relative to the position of impurity was not investigated.

In the presented paper we investigate the local distribution of spin-dependent current

for different positions of the cross section plane and local I-V curves of TMJ with single impurity and for random distribution of impurities inside the barrier. We adopted the free electron model with exchange splitting for ferromagnetic electrodes and used nonequilibrium Keldysh technique [9] for calculating of nonlinear on applied voltage transport properties.

We considered the model of TMJ as a three layers system, consisted from two thick ferromagnetic electrodes $\mathbb{F}$ separated by the insulating layer, $\mathbb{I}$. Inside the barrier the single nonmagnetic impurity with attracting potential was situated at some distance from $\mathbb{F}/\mathbb{I}$ interface. The two cases were investigated : parallel and antiparallel orientations of $\mathbb{F}$-layers magnetization.

The $\mathbb{F}$-electrodes are connected to the reservoirs with chemical potentials μ_1 and μ_2 so that $\mu_2 - \mu_1 = eV$, where V is the applied voltage.

To calculate the current through the system we have to found Keldysh Green function G^{-+} and advanced and retarded Green functions G^A and G^R. Solving the Dyson equation we found that

$$G^{-+}(\mathbf{r},\mathbf{r}') = G_0^{-+}(\mathbf{r},\mathbf{r}') + \frac{G_0^R(\mathbf{r},\mathbf{r}_0)WG_0^{-+}(\mathbf{r}_0,\mathbf{r}')}{1-WG_0^R(\mathbf{r}_0,\mathbf{r}_0)} + \frac{G_0^{-+}(\mathbf{r},\mathbf{r}_0)WG_0^A(\mathbf{r}_0,\mathbf{r}')}{1-WG_0^A(\mathbf{r}_0,\mathbf{r}_0)} + \frac{G_0^R(\mathbf{r},\mathbf{r}_0)WG_0^{-+}(\mathbf{r}_0,\mathbf{r}_0)WG_0^A(\mathbf{r}_0,\mathbf{r}')}{\left(1-WG_0^R(\mathbf{r}_0,\mathbf{r}_0)\right)\left(1-WG_0^A(\mathbf{r}_0,\mathbf{r}_0)\right)} \quad (1)$$

where $G_0^{-+}(\mathbf{r},\mathbf{r}'), G_0^A(\mathbf{r},\mathbf{r}')$ and $G_0^R(\mathbf{r},\mathbf{r}')$ are the Green's functions for the system in the absence of the impurity and the potential of the impurity V was represented as δ-function: $V(\mathbf{r}) = Wa_0^3\delta(z-z_0)\delta(\boldsymbol{\rho}\text{-}\boldsymbol{\rho_0})$, $\mathbf{r}_0 = (\boldsymbol{\rho_0}, z_0)$ is the position of the impurity, a_0 is it's effective radius, W is it's intensity. The explicit expressions for G^A, G^R, G^{-+} have the following form:

$$\begin{aligned} G_0^R(\mathbf{r},\mathbf{r}') = \int d^2\kappa \tfrac{(-1)\mathrm{e}^{-i\boldsymbol{\kappa}(\boldsymbol{\rho}-\boldsymbol{\rho}')}}{2\sqrt{q(z)q(z')}den} \left\{E(z_2,z)\left[q(z_2)+ik_2\right] + E^{-1}(z_2,z)\left[q(z_2)-ik_2\right]\right\} \\ \times\left\{E(z',z_1)\left[q(z_1)+ik_1\right] + E^{-1}(z',z_1)\left[q(z_1)-ik_1\right]\right\}, \end{aligned} \quad (2)$$

$$\begin{aligned} G_0^A(\mathbf{r},\mathbf{r}') = \int d^2\kappa \tfrac{(-1)\mathrm{e}^{i\boldsymbol{\kappa}(\boldsymbol{\rho}-\boldsymbol{\rho}')}}{2\sqrt{q(z)q(z')}den^*} \left\{E(z_2,z)\left[q(z_2)-ik_2\right] + E^{-1}(z_2,z)\left[q(z_2)+ik_2\right]\right\} \\ \times\left\{E(z',z_1)\left[q(z_1)-ik_1\right] + E^{-1}(z',z_1)\left[q(z_1)+ik_1\right]\right\}, \end{aligned} \quad (3)$$

$$
\begin{aligned}
&G_0^{-+}(\mathbf{r},\mathbf{r}') = \int d^2\kappa \frac{i4k_1 q(z_1) n_L \mathrm{e}^{-i\boldsymbol{\kappa}(\boldsymbol{\rho}-\boldsymbol{\rho}')}}{\sqrt{q(z)q(z')}|den|^2} \left\{E(z',z_2)\left[q(z_2)+ik_2\right]+E^{-1}(z',z_2)\left[q(z_2)-ik_2\right]\right\} \\
&\times \left\{E(z,z_2)\left[q(z_2)-ik_2\right]+E^{-1}(z,z_2)\left[q(z_2)+ik_2\right]\right\} \\
&+\int d^2\kappa \frac{i4k_2 q(z_2) n_R \mathrm{e}^{-i\boldsymbol{\kappa}(\boldsymbol{\rho}-\boldsymbol{\rho}')}}{\sqrt{q(z)q(z')}|den|^2} \left\{E(z_1,z')\left[q(z_1)+ik_1\right]+E^{-1}(z_1,z')\left[q(z_1)-ik_1\right]\right\} \\
&\times \left\{E(z_1,z)\left[q(z_1)-ik_1\right]+E^{-1}(z_1,z)\left[q(z_1)+ik_1\right]\right\},
\end{aligned}
\tag{4}
$$

where

$$q(z)=\sqrt{q_0^2+\kappa^2-\frac{2m}{\hbar^2}\frac{(z-z_1)}{(z_2-z_1)}eV},$$

$$k_1=\sqrt{\frac{2m}{\hbar^2}(\varepsilon-\Delta_1)-\kappa^2},$$

$$k_2=\sqrt{\frac{2m}{\hbar^2}(\varepsilon-\Delta_2+eV)-\kappa^2},$$

$$den=\left\{E(z_1,z_2)\left[q(z_2)-ik_2\right]\left[q(z_1)-ik_1\right]-E^{-1}(z_1,z_2)\left[q(z_2)+ik_2\right]\left[q(z_1)+ik_1\right]\right\},$$

$$E(z_1,z_2)\equiv \mathrm{e}^{\int_{z_1}^{z_2} q(\tau)d\tau},$$

$\boldsymbol{\kappa}$ is the electron momentum perpendicular to the plane of structure, ε is the energy, z_1 and z_2 are the positions of $\mathbb{F}/\mathbb{I}$ interfaces, Δ_1 and Δ_1 denote the positions of energy band bottom for spin up and down subbands.

$n_L = f^0(\varepsilon)$ and $n_R = f^0(\varepsilon+eV)$ are Fermi distribution functions in the left and right reservoirs and $\frac{\hbar^2 q_0^2}{2m}$ height of potential barrier above Fermi's level.

In (1),(2),(3) and (4) $\boldsymbol{\rho}$ and z are in the plane and perpendicular to the plane coordinates, and we consider that z and z_0 are situated within the barrier. We have to take into account that all Green functions are matrixes in spin space. We have consider $k_{1F}^{\uparrow}$, $k_{1F}^{\downarrow}$, $k_{2F}^{\uparrow}$, $k_{2F}^{\downarrow}$ are Fermi wave vectors of electron with spin$\uparrow$ ($\downarrow$) in the left and right $\mathbb{F}$-electrodes. The current was calculated, using the following expression:

$$j_z(\rho,z)=\frac{e\hbar}{2m}\int d\varepsilon\left(\frac{\partial G^{-+}(z,\rho;z',\rho)}{\partial z'}-\frac{\partial G^{-+}(z,\rho;z',\rho)}{\partial z}\right)_{z=z'} \tag{5}$$

On the Fig.1 and Fig.2 the dependencies of the currents in different channels (up and down spin) on coordinate $\rho-\rho_0$ at one interface $\mathbb{I}/\mathbb{F}$ ($z_2 = 15$Å) (another interface is at

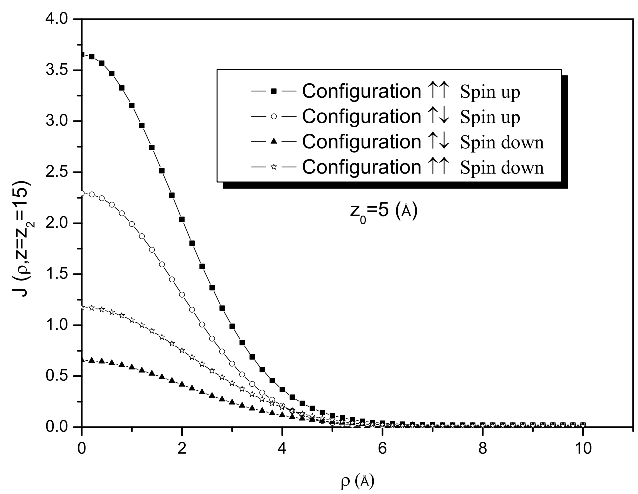

FIG. 1: Dependence of the current for different spin channels and P and AP configuration on the distance from the impurity in the plane of the structure at z=15 Å. $k_F^{\uparrow} = 1.1$ Å^{-1}, $k_F^{\downarrow} = 0.6$ Å^{-1}, $q_0 = 1.0$ Å^{-1}

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$z_1 = 0$) and inside the barrier at $z = 10$ are shown. Position of the impurity is at $\rho_0 = 0$ and $z_0 = 5$Å.

So in the vicinity of the impurity the hot spot of the radius approximately equal 6Å may be observed and the value of the current density in the center of the hot spot exceeds the value of the background current on several orders of magnitude. On the Fig.3 the TMR dependence on the distance from the impurity at different z is shown. It is interesting that the value of TMR in vicinity of the impurity exceeds it's background value (TMR for the ideal structure is equal 0.013) more over then order of magnitude and for some cases it exists the region of $\rho - \rho_0$ where TMR becomes negative.

Now on Fig.4 the I-V current for positive and negative applied voltage is shown. This curves are quite asymmetric on the sign of the voltage. It is connected with asymmetry of position of the impurity inside of the barrier. We choose the potential of impurity so that bound (resonance) state of electrons with spin up located near Fermi level for the positive applied voltage $= 1.2\ V$, and for negative voltage the position of this bound state lies below Fermi level. This diode behavior is demonstrated for the single impurity and to have the possibility to use this diode effect in practice we have to investigate the case of the finite

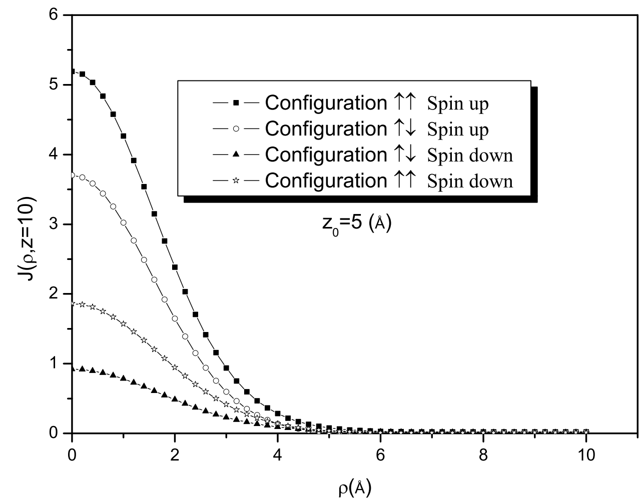

FIG. 2: The same dependence at $z = 10$ Å.

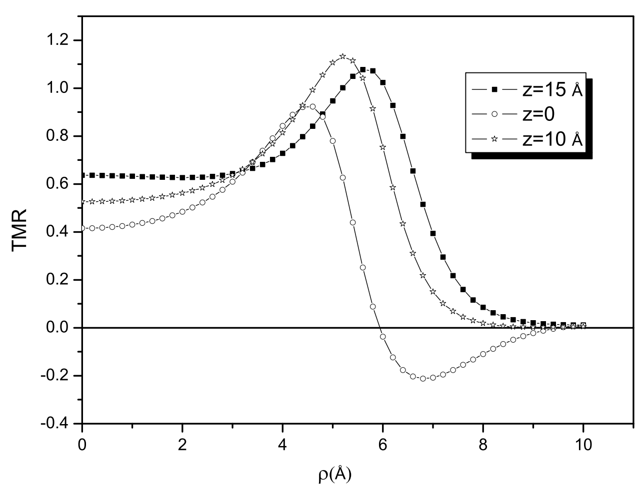

FIG. 3: Dependence of TMR on the distance from the impurity in the plane of the structure at different z. For parameters see Fig.1

concentration of impurities.

In this case we consider the same magnetic tunnel barrier structure with monolayer of impurities of finite atomic concentration x, situated closer to the one of $\mathbb{F}/\mathbb{I}$ interface. To solve the problem as a first step we have to find coherent potential and effective Keldysh Green function G_{eff}^{-+}. Solving the Dyson equation in the Keldysh space we got the following

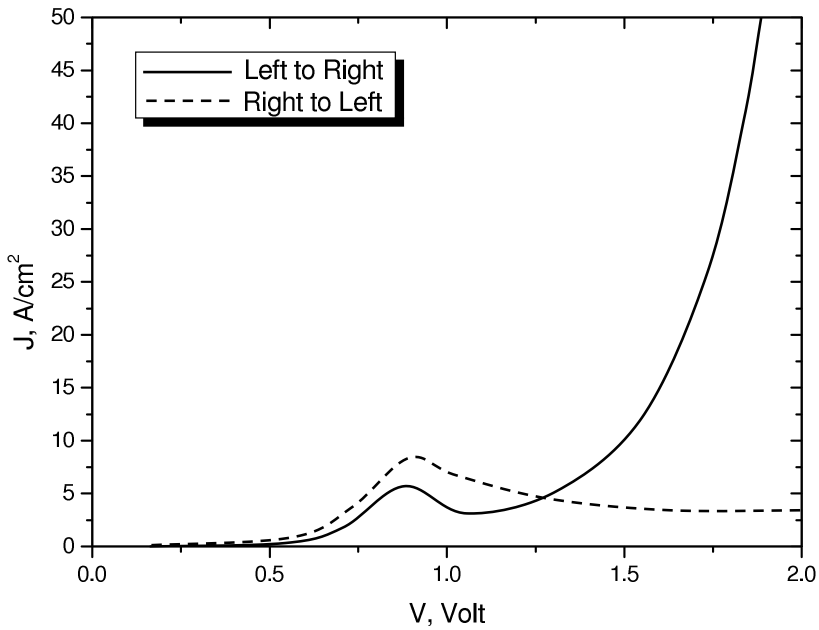

FIG. 4: Local I-V curve at $\rho = \rho_0$ and $z = 15$ Å for the case of single impurity.

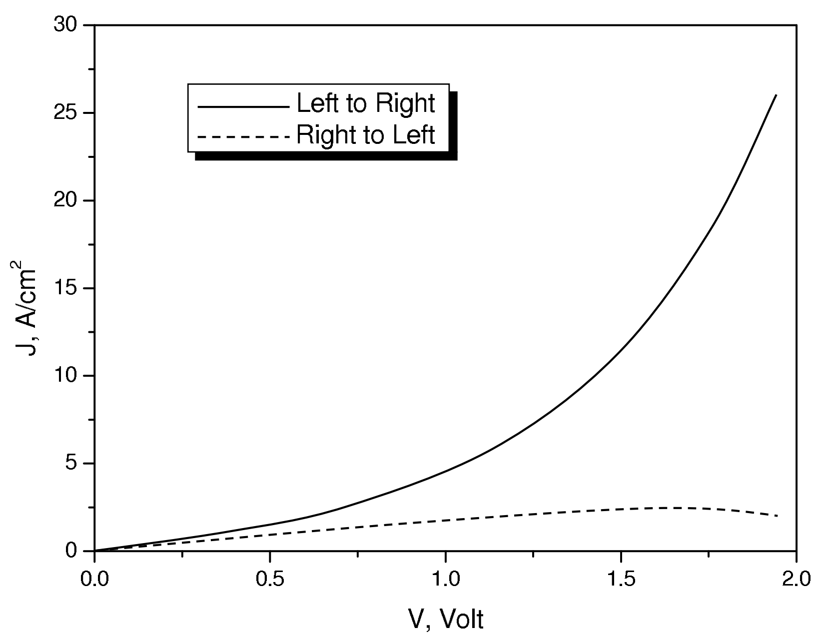

FIG. 5: I-V curve in the case of the layer of impurities at $z_0 = 3$Å and $x = 0.5$.

expression for $G_{\uparrow\uparrow}^{-+AP}$:

$$G^{-+}(z,z') = G_0^{-+}(z,z') + \frac{G_0^{-+}(z,z_0)\,\Sigma^A G_0^A(z_0,z')}{1 - G_0^A(z_0,z_0)\,\Sigma^A} + \frac{G_0^R(z,z_0)\,\Sigma^R G_0^{-+}(z_0,z')}{1 - G_0^R(z_0,z_0)\,\Sigma^R} - \frac{G_0^R(z,z_0)\,\Sigma^{-+} G_0^A(z_0,z')}{\left(1 - G_0^A(z_0,z_0)\,\Sigma^A\right)\left(1 - G_0^R(z_0,z_0)\,\Sigma^R\right)} + \frac{G_0^R(z,z_0)\,\Sigma^R G_0^{-+}(z_0,z_0)\,\Sigma^A G_0^A(z_0,z')}{\left(1 - G_0^A(z_0,z_0)\,\Sigma^A\right)\left(1 - G_0^R(z_0,z_0)\,\Sigma^R\right)} \quad (6)$$

where $\Sigma^{R(A)}$ are the coherent potential (C.P.) for the retarded and advanced Green functions,

which has to be found from the C.P.A equation:

$$\bar{t} = (1-x)\frac{(\varepsilon^A - \Sigma)}{1-(\varepsilon^A - \Sigma)G_{\text{eff}}(z_0,\rho_0;z_0,\rho_0)} + (x)\frac{(\varepsilon^B - \Sigma)}{1-(\varepsilon^B - \Sigma)G_{\text{eff}}(z_0,\rho_0;z_0,\rho_0)} = 0 \qquad (7)$$

where ε^A and ε^B are the onsite energies of the host (Al_2O_3) and the impurity (Al) and $\Sigma^{-+} = \frac{i}{2}(n_R + n_L)(\Sigma^R - \Sigma^A)$.

Now to calculate I-V curve we may use the found $G_{\alpha\alpha}^{-+P(AP)}$, substituting it into the expression (5).

On the Fig.5 the I-V curve for AP configuration is shown, and the asymmetry of the curve on the sign of applied voltage is clearly seen.

Such a structure may be prepared if to sputter thin layer of Al on the $\mathbb{F}$-electrode, then oxidise it, after sputter thicker layer of Al and oxidise it from the top side not completely. So some thin layer of the random alloy $Al_xAl_2O_{3(1-x)}$ is situated inside the more or less ideal insulator Al_2O_3 at the distance close to the first $\mathbb{F}/\mathbb{I}$ interface.

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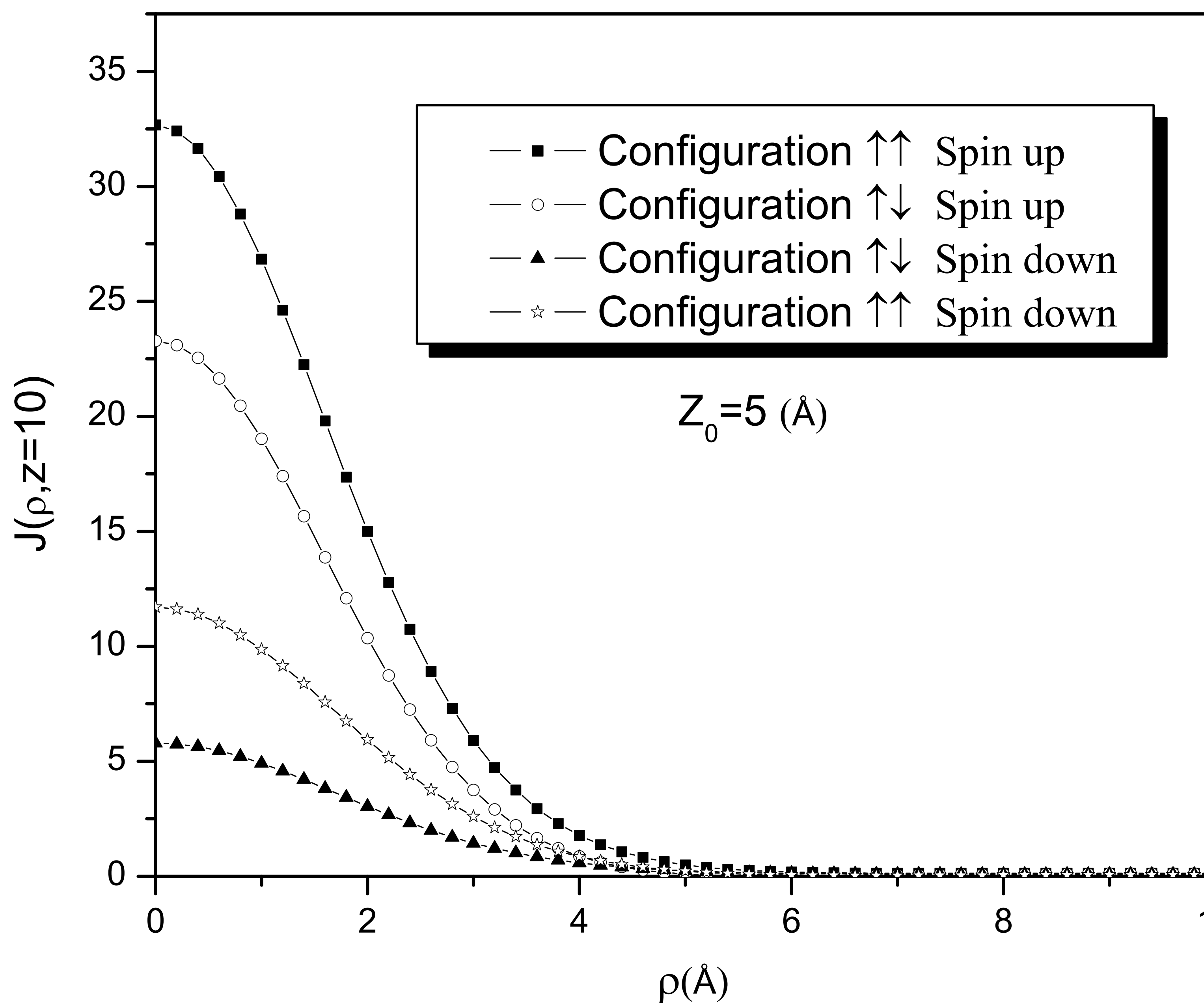
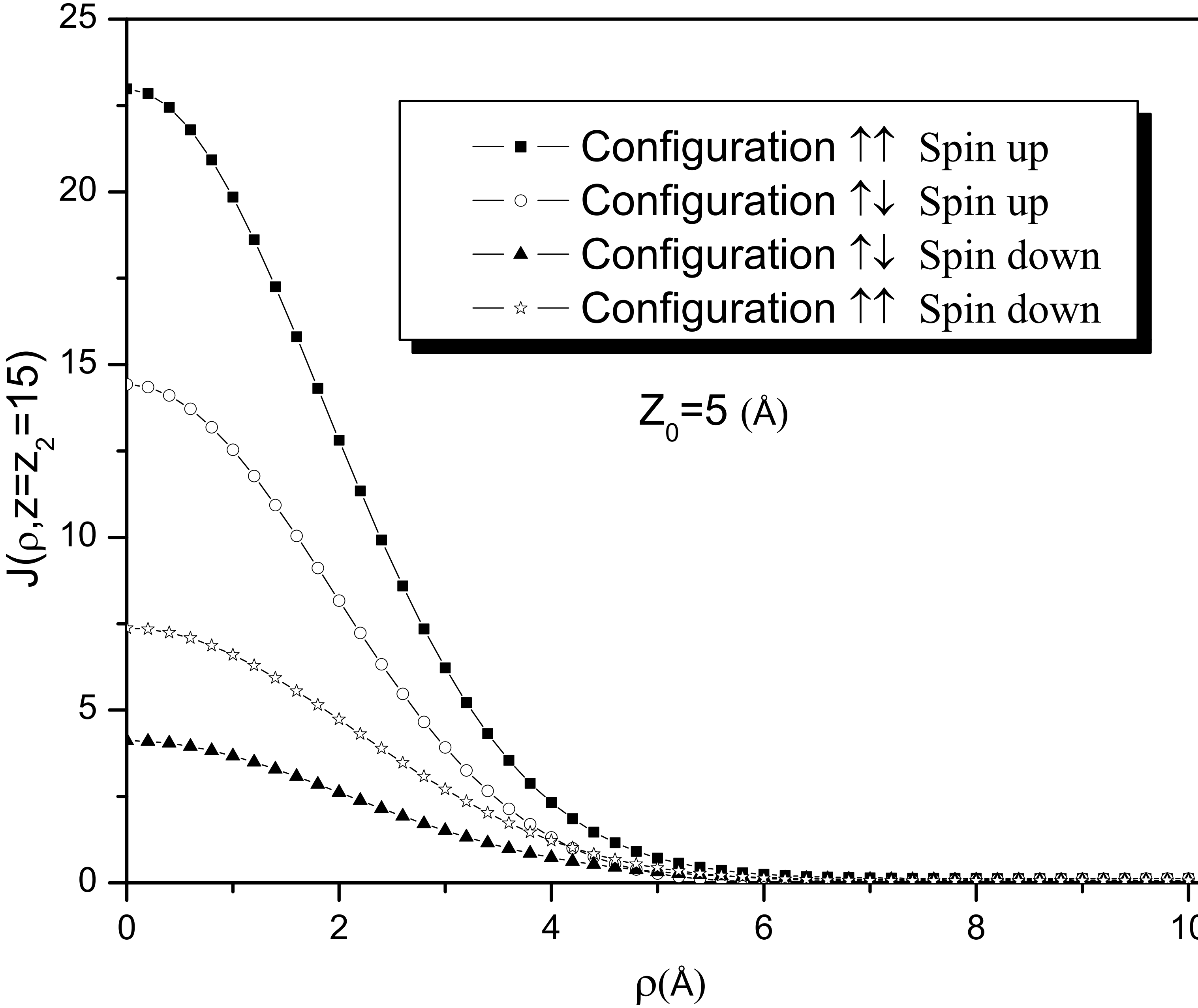


Configuration ↑↑ Spin up
Configuration ↑↓ Spin up
Configuration ↑↓ Spin down
Configuration ↑↑ Spin down
Z0=5 (Å)
J(ρ,z=10)
ρ(Å)
0
5
10
15
20
25
30
35
0
2
4
6
8



Configuration ↑↑ Spin up
Configuration ↑↓ Spin up
Configuration ↑↓ Spin down
Configuration ↑↑ Spin down
Z_0=5 (Å)
$J(\rho, z=z_2=15)$
ρ(Å)
0
5
10
15
20
25
0
2
4
6
8
10